# The effect of Cr concentration on single interstitials stability in FeCr alloys


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## Abstract

Finding adequate materials to withstand the demanding conditions in future fusion and fission reactors is a real challenge in the development of these technologies. Structural materials are going to be subjected to high irradiation doses and operating temperatures which will affect and modify material properties at a microstructural level. Understanding the changes in the microstructure induced by irradiation is needed in order to predict the response of these materials, ensuring safe and reliable future power plants. High-Cr ferritic/martensitic steels are preferred candidate structural materials due to their high resistance to radiation effects and their good resistance against corrosion. On the other hand, it is well known that these alloys present a problem of embrittlement, which could be caused by the presence of defects created by irradiation as these defects act as obstacles for dislocation motion. Therefore, the mechanical response of these materials will depend on the type of defects created during irradiation. In this work, we address a study of the effect of Cr concentration on single interstitial defect formation energies in FeCr alloys.


## Methodology

Molecular static calculations with the CD-EAM empirical potential[1,2]. Calculations are performed for <111>, <110> and <100> self- and mixed-interstitials with a cell size of 2001 atoms and placing an interstitial at all possible lattice sites of the supercell. Cr concentrations range from 1 to 17%. Code: LAMMPS.

## Results and Discussion

### Cr concentration effect:

- 2000 calculations for each concentration.
- The final configuration after optimization has been analyzed to check if it has the same crystallographic orientation and character (FeFe, FeCr) as the original one. Only those cases where the initial and final configurations are the same are considered. Initial interstitial atoms considered are FeFe and FeCr in three configurations: <100>, <110> and <111>

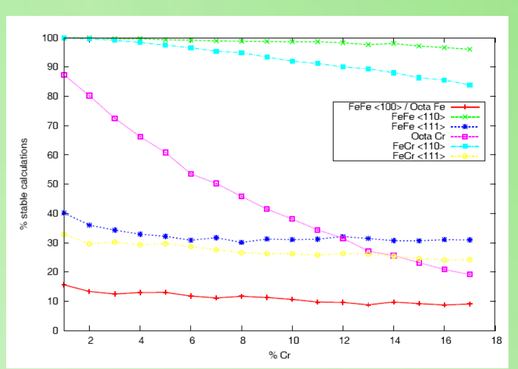



**Figure 1. Percentage of configurations that do not change geometry or character used in the calculation of average formation energy of figure 2.**

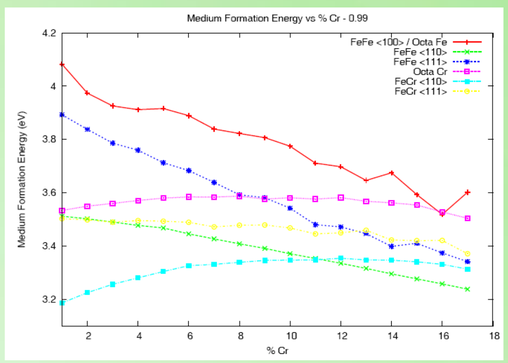
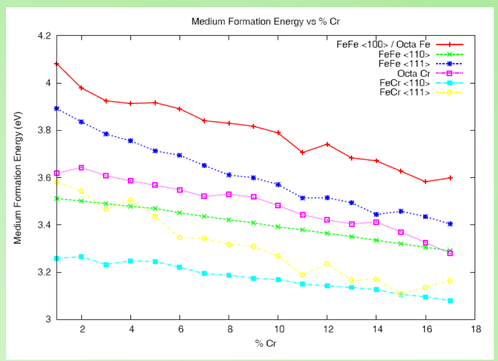



**Figure 2. Average formation energy of the different configurations as a function of Cr concentration. The interstitial is placed at all possible lattice sites of the supercell.**

- **Figure 3. Average formation energy of the different configurations as a function of Cr content. The interstitial is created so that the local concentration does not change: the interstitial atom is always an Fe atom and depending on the type of interstitial (FeFe or FeCr) an Fe or Cr atom is displaced from its equilibrium position in the cell.**



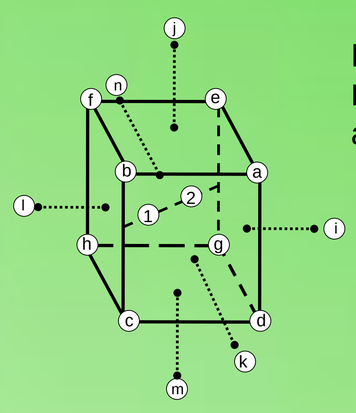

### Local Cr distribution effect:

- Calculation of formation energies of FeFe <110> and FeCr <110> in an Fe sample when changing the local environment: one Cr atom at different first and second nearest neighbors.

| $Cr_{subst}$ | $E_f$ | $D_{Cr\ subst-2}$ |
|---|---|---|
| **a, e** | 3.47 | 0.722 |
| **c, h** | 3,47 | 1.302 |
| **d, g** | 3.41 | 0.927 |
| **b, f** | 3.41 | 0.927 |
| **i, j** | 3.49 | 0.766 |
| **l, m** | 3.49 | 1.318 |
| **k, n** | 3.52 | 1.031 |

$E_f$ = 3.52 eV
$D_{1-2}$ = 0.736
$D_{2-a} = D_{2-e}$ = 0.763
$D_{2-d} = D_{2-g}$ = 0.923
$D_{2-b} = D_{2-f}$ = 0.923
$D_{2-c} = D_{2-h}$ = 1.317
$D_{2-i} = D_{2-j}$ = 0.817
$D_{2-k} = D_{2-n}$ = 1.053
$D_{2-l} = D_{2-m}$ = 1.322

② Fe atom




$D_{1-2}$ = distance between interstitial atoms
$D_{Cr\ subst-2}$ = distance between the interstitial atom 2 and the Cr atom at the substitution position, i.e. a, b, c, d, e, f, g, h, i, j, k, l, m, or n

| $Cr_{subst}$ | $E_f$ | $D_{Cr\ subst-2}$ |
|---|---|---|
| **a, e** | 4.16 | 0.801 |
| **c, h** | 3,46 | 1.306 |
| **d, g** | 3.57 | 0.970 |
| **b, f** | 3.57 | 0.971 |
| **i, j** | 3.73 | 0.878 |
| **l, m** | 3.46 | 1.361 |
| **k, n** | 3.60 | 1.052 |

② Cr atom

$E_f$ = 3.16 eV
$D_{1-2}$ = 0.713
$D_{2-a} = D_{2-e}$ = 0.729
$D_{2-b} = D_{2-f}$ = 0.931
$D_{2-d} = D_{2-g}$ = 0.931
$D_{2-h} = D_{2-c}$ = 1.317
$D_{2-i} = D_{2-j}$ = 0.813
$D_{2-k} = D_{2-n}$ = 1.045
$D_{2-l} = D_{2-m}$ = 1.328

$$E_f = E_{defect} - (E_{without\ defect} + A) \quad \text{where} \quad A = E(Fe) \text{ or } E(Cr)$$

$E_f$ = Formation energy of the defect
$E_{defect}$ = Energy of the cell with a defect
$E_{without\ defect}$ = Energy of the cell without a defect
**E(Fe)** = Perfect energy of the Fe (FeFe interstitial) per atom
**E(Cr)** = Perfect energy of the Cr (FeCr interstitial) per atom

## Conclusions

- The most probable and stable geometry is <110> comparing with <100>/Octa and <111> geometries.
- For Cr concentrations higher than 10% a change in the stability is observed: self-interstitials are more stable than mixed-interstitials for <110> and <111> geometries.
- If only configurations with the same local Cr concentration are taken into account, mixed-interstitials are always the more stable ones. So, the change in stability observed when the interstitial is placed at all possible lattice sites of the supercell (Fig. 2) it is due to the increase of Cr content, not because of a higher stability of the interstitial.
- The local Cr distribution study shows that:
  - Formation energy depends strongly on Cr position for the case of FeCr <110> interstitials and weakly in the case of FeFe <110> interstitials.
  - The shorter the distance between Cr atoms, the greater the formation energy

## References


[1] A. Caro, D.A. Crowson, M. Caro Phys. Rev. Lett.95 (2005**)** 075702.

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